APPENDIX A
DESCRIPTION AND OUTPUT OF A COMMODITY FLOW ALLOCATION MODEL (SRI International, 1993)

A.1 DESCRIPTION OF THE COMMODITY FLOW ALLOCATION MODEL

A commodity flow allocation model was used by SRI International to assign hazardous chemical flows between producers and consumers. The model is a modified gravity model based on the premise that the shorter the distance between an origin-destination pair (e.g., a chemical production facility and a consumer of that chemical), the greater the likelihood of cargo flow between that pair. In this study, the following assumptions were used in the implementation of the gravity model:

- Available supply at each origin (e.g., production location) was set equal to the net production available for truck shipments.
- The total amount demanded at each destination was set equal to the estimated demand for truck delivery.
- The impedance relation was modified to reflect corporate affiliations (captive consumers) and possible use of terminal facilities.
- After discussions with chemical producers, it was discovered that some consuming plants, as a matter of policy, do not purchase from specified companies. For these cases, the flow between origin and destination was set to zero.

To estimate the highway distances between origins and destinations and highway routes used by trucking companies, an off-the-shelf software package called PCMiler is used. PCMiler identifies the minimum distance between two points for specified types of highway (e.g., interstates). ZIP codes were used to identify the locations of producing and consuming plants.

The unaltered gravity model has a tendency to attempt to assign at least a small increment of flow to all possible origin-destination pairs. In reality, such small commodity flows do not occur. The model, therefore, truncates all flows below a minimum threshold value and sets the cell value to zero. The minimum threshold was set equal to 20 tons per year (e.g., the approximate weight of one average-sized bulk truck load per year).

A.2 OVERVIEW OF CHEMICALS STUDIED

Using a generalized gravity flow model, SRI developed a list of 147 large-volume chemicals that account for at least 80% of U.S. truck shipments of hazardous chemicals. Exhibit A-1 lists these chemicals and their estimated production volumes, in decreasing order. Three chemicals were selected for detailed analysis using the model: 1-butanol, dodecene-1, and phosphorus pentasulfide. In the next subsections, brief overviews of the characteristics, uses, and geographical distribution of producers and consumers are presented.

A.2.1 1-Butanol

1-Butanol, which appears in the top one-third of the chemicals listed in Exhibit A-1, is a low-boiling liquid classified as a fire or explosion and health hazard (Guide No. 26 in the DOT Emergency Response Guidebook [ERG]). The chemical is principally used for the production of methacrylate esters, glycol ethers, and butyl acetate, as well as direct use as a solvent.

DOT Emergency Response Guidebook (ERG). The ERG is not a regulatory guide, but is designed for the sole purpose of aiding emergency responders in the initial phases of an incident.

U.S. production of 1-butanol in 1987 is estimated at 575,000 short tons, of which 450,000 short tons was available for shipment to off-site consumers. All production is in the Texas-Louisiana region, while consumption of the chemical is concentrated in the Chicago, Illinois, New Jersey, and Los Angeles, California areas. There are six producers (five of which have terminals) and 67 major consuming plants.

1-Butanol is shipped by barge, rail, and truck. Most large volume shipments of 1-butanol are made by barge using inland and coastal waterways. Rail shipments are used for large volume movements that do not follow navigable waterways. Truck movements tend to be limited to short haul (i.e., from a terminal to the end-user) or small volume shipments in drums. Companies using 1-butanol as a solvent have it delivered by truck in mixed shipments using compartmented tankwagons or cargo tank trucks. Most tankwagon shipments originate from terminals located near major consuming centers. It is estimated that 83,200 short tons are delivered annually by truck.

A.2.2 Dodecene-1

Dodecene-1, with an estimated 1987 production of 200,000 short tons, is in the middle third of the list of 147 chemicals. It is a high-boiling liquid identified as propylene tetramer and is classified as a fire, explosion, and health hazard (Guide No. 27 in the DOT ERG). Consumption of dodecene-1 is primarily for the production of branched dodecylbenzene, tridecyl alcohol, and dodecylphenol.

Because dodecene-1 is used in the manufacture of other chemicals at its producing plants, the quantities used in captive production are not available for shipment elsewhere. Of the plants producing dodecene-1, four were identified as net producers that ship their product domestically, either directly from their plant or from terminals supplied by barge or other ocean-going vessels. Several additional production plants were eliminated from the analysis because contacts in the industry confirmed that no product was available for off-site shipment by highway.

Thirteen plants were identified as net consumers of the chemical, and of these only eight received shipments by truck. An estimated 15,100 tons are shipped by highway.

A.2.3 Phosphorus Pentasulfide

Phosphorus pentasulfide, with an estimated U.S. production of 70,000 short tons in 1987, is in the lower third of the list of chemicals given in Exhibit A-1. It is a high-melting solid that may ignite in the presence of moisture and produce poisonous gas, as identified in DOT ERG Guide No. 41. Phosphorus pentasulfide is used primarily for production of pesticides and lubricating oil additives. Production and consumption are widely distributed from the Northeast to the Southeast.

Four plants produce phosphorus pentasulfide, and thirteen plants are identified as net consumers of phosphorus pentasulfide. Most consuming plants are located in the Mid-Atlantic and Southern states, and the producing plants are in Illinois, Kansas, Pennsylvania, and Tennessee. One of the consuming plants receives shipments exclusively by rail, and the remaining twelve have an estimated demand of 52,500 tons.

EXHIBIT A-1
LIST OF 147 LARGE VOLUME CHEMICALS

Chemical	Production Volume, 1987 (thousands of Short Tons)	Chemical	Production Volume, 1987 (thousands of Short Tons)
Sulfuric Acid	39,235	Acrylic Acid	550
Propane	26,896	Hexamethylenediamine	543
Nitrogen	24,515	Isobutylene	518
Oxygen	16,669	Hydrogen Cyanide	516
Ammonia	16,100	Methyl Methacrylate	514
Calcium Oxide	15,733	Phthalic Anhydride	508
Sodium Hydroxide	11,486	O-Xylene	470
Chlorine Gas	11,019	Methylene-Diphenylene Diisocyanate	467
Phosphoric Acid	10,685		
Sulfur	10,321	Cyclohexanone	465
Carbon Dioxide	8,307	Barite	448
Ethylene Dichloride	7,878	Aniline	430
Ammonium Nitrate	7,612	Hexane	426
Nitric Acid (100% HNO_3 Basis)	7,225	Phosgene	421
Benzene	5,904	Linear Alkylate Sulfonate	399
Ethylbenzene	4,630	Hydrogen	389
Vinyl Chloride	4,201	Carbon Tetrachloride	374
Styrene	4,007	Acetaldehyde	363
Methanol	3,769	Toluene Diisocyanate	357
Toluene	3,223	Methylchloroform	347
Ethylene Oxide	2,921	Phosphorus	344
Hydrochloric Acid (100%)	2,869	Methyl Ethyl Ketone	336
P-Xylene	2,578	Sodium Chlorate	289
Methyl-T-Butyl Ether	1,757	Tripropylene (Nonene)	275
Phenol	1,676	Hydrofluoric Acid	274
Acetic Acid, Synthetic	1,623	Methyl Chloride	261
1,3-Butadiene	1,465	Methylene Dichloride	259
Ethanol (Synthetic)	1,434	N-Butyl Acrylate	258
Aluminum Sulfate	1,426	Potassium Hydroxide	246
Carbon Black (Furnace Black)	1,362	Perchloroethylene	237
Vinyl Acetate	1,253	1-Butene	231
Acrylonitrile	1,250	Calcium Carbide	230
Formaldehyde	1,232	Sulfur Dioxide	229
Cyclohexane	1,137	Epichlorohydrin	225
Propylene Oxide	1,105	Chloroform	224
Acetone	1,048	Propylene Tetramer (Dodecene)	200
Butyraldehyde	879	Maleic Anhydride	193
Acetic Anhydride	858	Dichlorodifluoromethane (F12)	184
Adipic Acid	795	Acetylene	182
Isopropanol	685	Carbon Disulfide	180
Nitrobenzene	625	Ethylene Glycol Monobutyl Ether	175
1-Butanol	575	Bromine	168
Argon	560	Ethyle Acrylate	162

EXHIBIT A-1
LIST OF 147 LARGE VOLUME CHEMICALS
(Continued)

Chemical	Production Volume, 1987 (thousands of Short Tons)	Chemical	Production Volume, 1987 (thousands of Short Tons)
Hydrogen Peroxide	153	Isoprene	54
Chlorodifluoromethane (F22)	142	Zinc Sulfate	54
N-Pentane	142	Ethylene Glycol Monoethyl Ether	53
Propionaldehyde	140		
Ferric Chloride	137	P-Dichlorobenzene	52
Nonylphenol	137	Dicyclopentadiene	50
Sodium Chromate/Dichromate	128	Hydrofluosilicic Acid	50
Chlorobenzene	123	Benzoic Acid	48
Naphthalene	121	Isobutyl Acetate	44
Monoethanolamine	116	Atrazine	43
Activated Carbon	109	Ethylene Glycol Monoethyl Ether Acetate	42
Ethyl Acetate	107		
Phosphorus Trichloride	102	Ethylenediamine Tetraacetic Acid	41
N-Butyl Acetate	101	Furfural	40
Isobutyraldehyde	99	Sodium Hydrosulfide	40
Trichloroethylene	98	Ethylenediamine	39
N-Propanol	93	Dimethylamine	37
Barium Sulfide	92	Cupric Sulfate	36
N-Heptane	89	Ethylene Glycol Monomethyl Ether	36
Calcium Hypochlorite	88	N-Propyl Acetate	35
Sodium Cyanide	85	Aluminum Chloride	33
Isobutanol	83	Benzyl Chloride	33
Pinene	78	Phosphorus Oxychloride	31
Sodium Hydrosulfite	78	Ethylene Dibromide	30
Ethyl Chloride	77	Zinc Chloride	28
Tetrahydrofuran	77	Isopropyl Acetate	27
Methyl Isobutyl Ketone	76	Isopropylamine, Mono	27
Chloronitrobenzene	73	Methylamine	26
Sodium (Metal)	72	Sodium Phosphate, Tribasic	26
Phosphorus Pentasulfide	70	Amyl Alcohol	25
Hexene-1	61		
Propionic Acid	59	**Total for 147 Chemicals**	**288,792**
Acrylamide	56		
Chlorinated Isocyanurates	55		

A.3 PRESENTATION OF RESULTS

For each of the chemicals studied, a map of the United States presenting the results of the commodity flow allocation model is attached (see Exhibit A-2, A-3, and A-4). These results are preliminary only and may differ significantly from the final results, which will be presented in subsequent reports on each of the three chemicals. GisPlus Map software, developed by the Caliper Corporation of Newton, Massachusetts, was used to prepare the maps. Two kinds of input data are used to produce the maps: point (node) and line (flow) files. The point data file provides the ZIP code location and descriptors for each of the producing and consuming plants. The link file provides the estimated flow (tonnage) of chemicals moving from each producing plant to each consuming plant.

GisPlus has an auxiliary database that contains descriptors of each of the nation's roads and highways. The descriptors include such items as local, state, or Federal control; paved or unpaved; all year or seasonal operating conditions; and height or weight restrictions. The maps produced assume that hazardous chemicals are not moved on certain types of roads, including restricted, unpaved, or seasonal roads. The GisPlus program tends to select larger, interstate routes, and avoid smaller, winding roads. In addition to the national maps presented in the exhibits, the software is capable of producing maps for individual states, counties, or other specified regions.

A.3.1 1-Butanol

Approximately 30,243 ton-miles of 1-butanol shipments are estimated (see Exhibit A-2). Because a combination of rail and truck shipment is generally less expensive than truck shipments alone, only about 12% of truck movements are estimated to originate at producing plants. Of the total ton-miles travelled, over 40% are accounted for in states where consumption from off-site sources is concentrated, such as California, Illinois, Michigan, and North Carolina. States in which production occurs (Texas and Louisiana) have little if any off-site consumption but capture about 20% of highway miles because of direct deliveries to other states. Only a few states with neither production or consumption facilities are shown to have any truck shipments. These states include Indiana, Arizona, and New Mexico.

A.3.2 Dodecene-1

Of the estimated 11,616 ton-miles of dodecene-1 moved by truck in 1987, nearly 20% occurred in Texas, a major consuming and producing state (see Exhibit A-3). About 14% of ton-miles occurred in Pennsylvania, a state that has neither production nor major consumption facilities. An additional 10% of total ton-miles occurred in Ohio, which has a production facility and a consuming plant that receives 15% of the estimated truck shipments of the chemical. Other states with neither production nor consumption facilities that have relatively large percentages of ton-miles include Alabama, Louisiana, Mississippi, Oklahoma, Tennessee, and Virginia. Because the volume of production and consumption of dodecene-1 is relatively small, terminal facilities have not generally been established to offset the cost of truck movements.

A.3.3 Phosphorus Pentasulfide

Because of the dispersed nature of production and consumption, and the heavy reliance on truck transport, there were an estimated 27,472 ton-miles of phosphorus pentasulfide moved by truck in 1987 (see Exhibit A-4). Nearly a quarter of the ton-miles are in Pennsylvania, a state with a production plant. Other states with about 10% to 15% of ton-miles are Ohio, Illinois, Indiana, Missouri, and Mississippi. Most of these states have either a production or consumption facility.

EXHIBIT A-2

1-BUTANOL FLOWS BY HIGHWAY

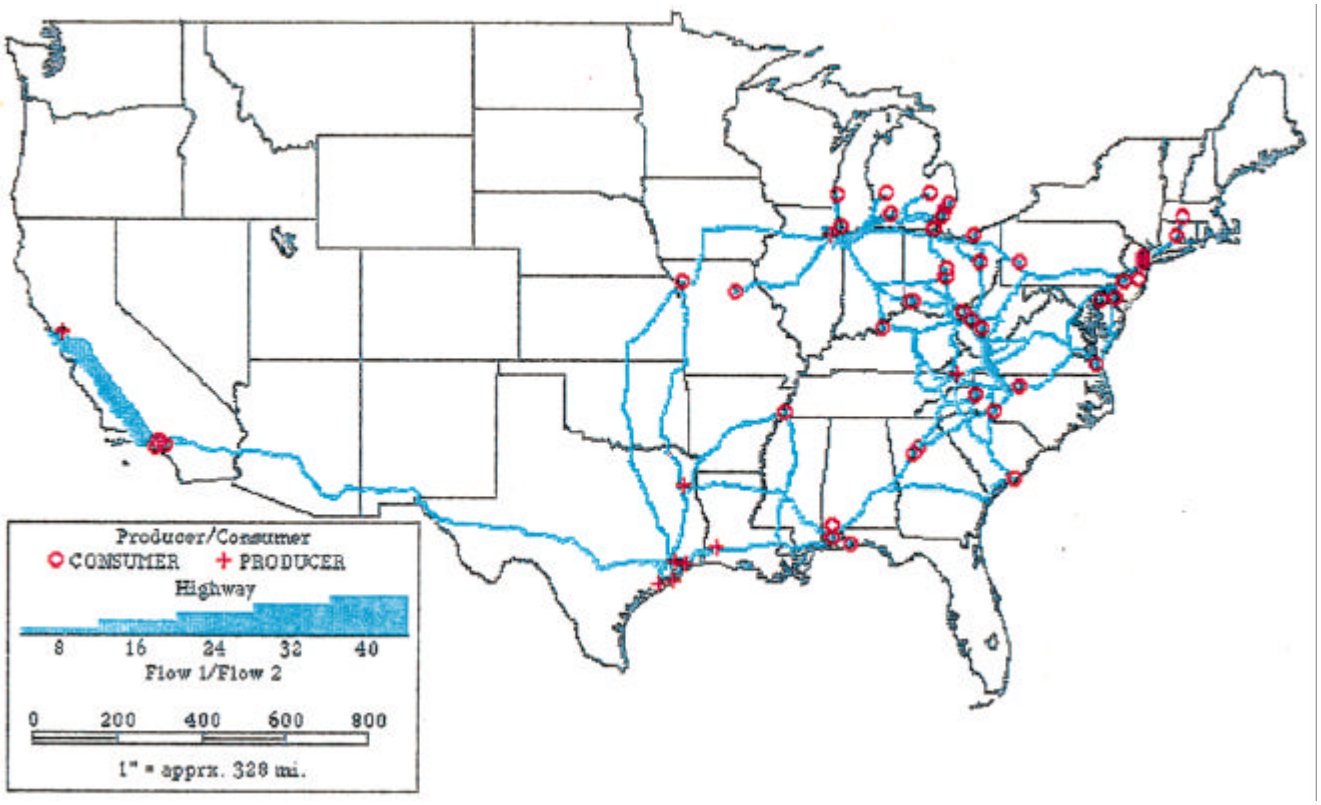

EXHIBIT A-3

DODECENE-1 FLOWS BY HIGHWAY

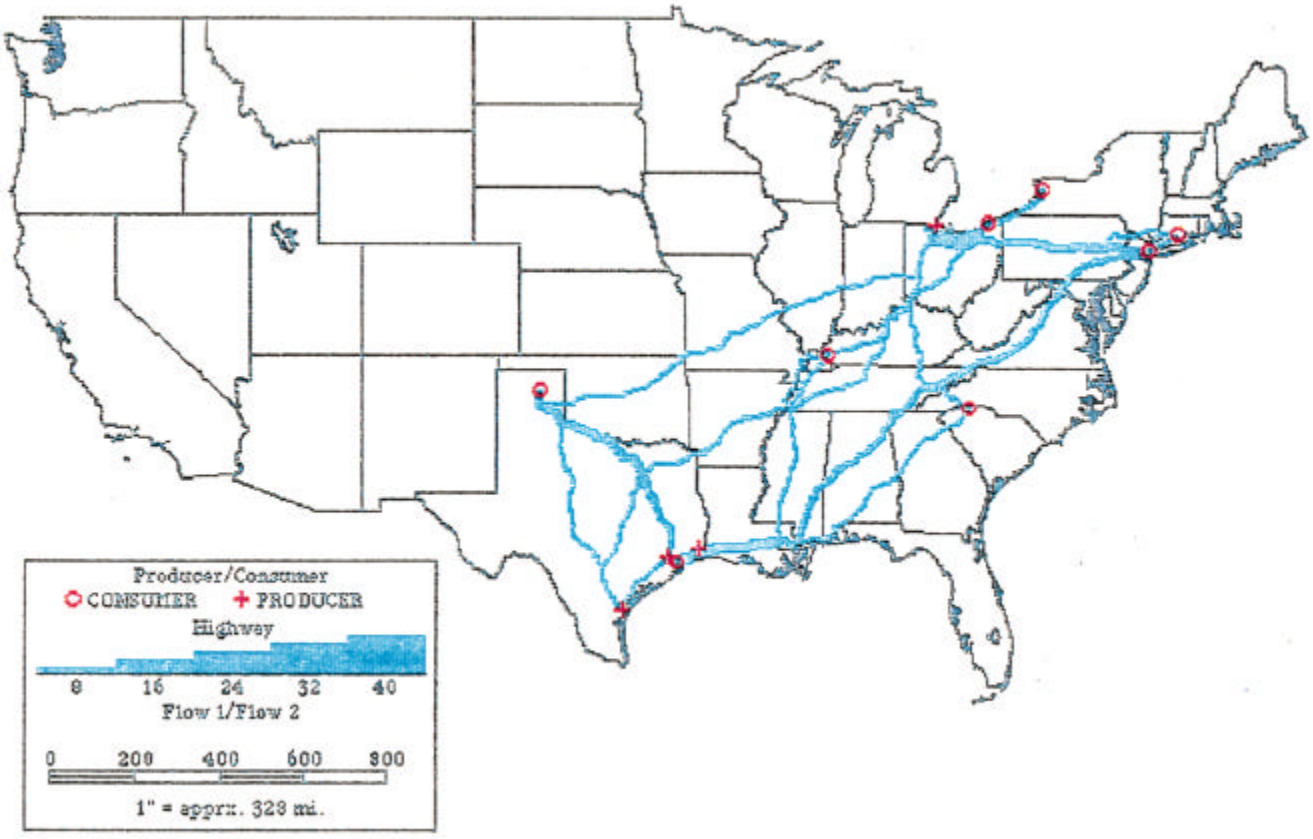

EXHIBIT A-3

DODECENE-1 FLOWS BY HIGHWAY